

Exact Results of Strongly Correlated Systems at Finite Temperature *

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Abstract

Some rigorous conclusions of the Hubbard model , Kondo lattice model and periodic Anderson model at finite temperature are acquired employing the fluctuation-dissipation theorem and particle-hole transform. The main conclusion states that for the three models, the expectation value of $\tilde{\mathbf{S}}^2 - \tilde{S}_z^2$ will be of order N_Λ at any finite temperature .

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Hubbard model(HM), Kondo lattice model (KLM) and periodic Anderson model (PAM) are three typical strongly-correlated electrons systems under currently intensive investigations. They exhibit unusual thermodynamic, magnetic and transport propertities (high- T_c) [1]-[16]. Dispite their superficial simplicities, exact results about them are unusually difficult to obtain in more than one

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dimensions [17]. Fortunately, a series of rigorous results about the ground state of the three models have been acquired [1]-[16]. To understand the magnetic properties of the ground state of the models, the reflection symmetry, or up-down symmetry is often employed and this method was initially utilized by Lieb[1]. Having knowing some features in the ground states, one is expecting some exact knowledge of the model at *finite* temperature. Apart from the various magnetic properties of the models, an extremely interesting feature is that it may provide an understanding of the high- T_c superconducting supported by cuprates such as YBaCuO. To investigate this aspect, one often utilizes the concept of off-diagonal long-range order (ODLRO) proposed by Yang as early as thirty years ago[18]. In [18], Yang showed that the existence of ODLRO of fermionic systems imply Bose-Einstein condensation. This relationship was made more clearer recently[19][20]. It is indeed supported by the BCS trial state, which does not nevertheless belong to the Hilbert space of the original Hamiltonian. Using the symmetry of the Hubbard model and η -pairing, Yang constructed many eigenstates of the Hamiltonian supporting ODLRO[2]. Later, Essler *et.al.* showed that the ground states of a couple of generalized Hubbard models possess ODLRO[4][6]. Though it is generally considered that the Hubbard model may account for the high- T_c enigma, the Kondo lattice model and periodic Anderson model are also possibly relevant because the superconducting properties are doping-dependent according to experiments.

In this letter, we make use of the fluctuation- dissipation theorem to study the pseudo-spins of the three models at finite temperature. The prototype one-band Hubbard model on a lattice Λ

$$H_{\text{HM}} = \sum_{(ij)} \sum_{\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

where $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are the creation and annihilation operators of the electrons with spin $\sigma = \uparrow, \downarrow$ at site i . The hopping matrix $\{t_{ij}\}$ are required to be real and symmetric. The number operators are $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$, while the U denotes the on-site Coulomb interaction. It is further assumed that the lattice Λ is bipartite in the sense that it can be divided into sublattices \mathbf{A} and \mathbf{B} , i.e. $\Lambda = \mathbf{A} \cup \mathbf{B}$, such that $t_{ij} = 0$ whenever $\{ij\} \in \mathbf{A}$ or $\{ij\} \in \mathbf{B}$. The Kondo lattice model is

$$H_{\text{KLM}} = \sum_{(ij)} \sum_{\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + J \sum_i \mathbf{S}_i^{\text{loc}} \cdot \mathbf{S}_i^c \quad (2)$$

where \mathbf{S}^{loc} are the localized spins of the impurities and \mathbf{S}^c are the spins of the conduction electrons (whose definition will be given later). This model can be clearly regarded as a doped Hubbard model.

The periodic Anderson model is described by

$$H_{\text{PAM}} = \sum_{(ij)} \sum_{\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i\sigma} \epsilon_f n_{i\sigma}^f + V \sum_{i\sigma} (c_{i\sigma}^{\dagger} f_{i\sigma} + f_{i\sigma}^{\dagger} c_{i\sigma}) + U_f \sum_i n_{i\uparrow}^f n_{i\downarrow}^f \quad (3)$$

where $n_{i\sigma}^f = f_{i\sigma}^{\dagger} f_{i\sigma}$ are the number operators of the localized electrons. Note that we have assumed that the conduction electrons have also on-site Coloumb interaction in both the Kondo lattice model and the periodic Anderson model. When $U = 0$, the model H_{PAM} is called *symmetric* if $2\epsilon_f + U_f = 0$. Here $U \neq 0$, we call the model symmetric if $2\epsilon_f + U_f = U$ and we consider this case only.

For HM and KLM the spin \mathbf{S}_c and pseudo-spin $\tilde{\mathbf{S}}_c$ for the conduction electrons, which is equivalent to the η -pairing, are defined as follows

$$S_c^+ = \sum_{i \in \Lambda} c_{i\uparrow}^{\dagger} c_{i\downarrow}, S_c^- = \sum_{i \in \Lambda} c_{i\downarrow}^{\dagger} c_{i\uparrow}, S_c^z = \frac{1}{2} \sum_{i \in \Lambda} (c_{i\uparrow}^{\dagger} c_{i\uparrow} - c_{i\downarrow}^{\dagger} c_{i\downarrow}) = \frac{1}{2} (N_{\uparrow} - N_{\downarrow}) \quad (4)$$

$$\tilde{S}_c^+ = \sum_{i \in \Lambda} \epsilon(i) C_{i\uparrow} c_{i\downarrow}, \quad \tilde{S}_c^- = \sum_{i \in \Lambda} \epsilon(i) c_{i\downarrow}^{\dagger} c_{i\uparrow}^{\dagger}, \quad \tilde{S}_c^z = \frac{1}{2} \sum_{i \in \Lambda} (1 - n_{i\uparrow} - n_{i\downarrow}) \quad (5)$$

where $\epsilon(i) = 1$ when $i \in \mathbf{A}$ and -1 when $i \in \mathbf{B}$. Both the spin and the pseudo-spin operators constitute SU(2) algebra and they commute with each other, i.e. $[\tilde{\mathbf{S}}_c, \mathbf{S}_c] = 0$, so they form an SU(2) \otimes SU(2) algebra. For HM, the total spin is $\mathbf{S} = \sum_i \mathbf{S}_i^c$ while for KLM, the total spin is $\mathbf{S} = \sum_i (\mathbf{S}_i^c + \mathbf{S}_i^{\text{loc}})$. It is not difficult to show that $[H, \tilde{\mathbf{S}}^2] = [H, \mathbf{S}^2] = [H, \tilde{S}_z] = [H, S_z] = 0$. Even, we have $[H, \mathbf{S}] = 0$ (but $[H, \tilde{\mathbf{S}}] \neq 0$ and $[H_{\text{KLM}}, \mathbf{S}_c] \neq 0$), $H = H_{\text{HM}}, H_{\text{KLM}}$. So both HM and KLM enjoy SU(2) \otimes U(1) \otimes U(1) symmetry. The spin is relevant to the magnetic properties while the pseudo-spin is relevant to superconducting. For HM, Yang and Zhang[3] showed that ODLRO exists whenever the expectation value of $\tilde{\mathbf{S}}^2 - \tilde{S}_z^2$ is of order N_{Λ}^2 , where N_{Λ} is the number of the sites of the lattice considered.

For PAM, the spin operators and pseudo-spin operators are[13]

$$S^+ = \sum_i (c_{i\uparrow}^{\dagger} c_{i\downarrow} + f_{i\uparrow}^{\dagger} f_{i\downarrow}), \quad S^- = \sum_i (c_{i\downarrow}^{\dagger} c_{i\uparrow} + f_{i\downarrow}^{\dagger} f_{i\uparrow}) \quad (6)$$

$$S^z = \frac{1}{2} \sum_i (c_{i\uparrow}^{\dagger} c_{i\uparrow} - c_{i\downarrow}^{\dagger} c_{i\downarrow} + f_{i\uparrow}^{\dagger} f_{i\uparrow} - f_{i\downarrow}^{\dagger} f_{i\downarrow}) \quad (7)$$

$$\tilde{S}^+ = \sum_i (-1)^i (c_{i\uparrow}^{\dagger} c_{i\downarrow} - f_{i\uparrow}^{\dagger} f_{i\downarrow}), \quad \tilde{S}^- = \sum_i (-1)^i (c_{i\downarrow}^{\dagger} c_{i\uparrow}^{\dagger} - f_{i\downarrow}^{\dagger} f_{i\uparrow}^{\dagger}) \quad (8)$$

$$\tilde{S}^z = \frac{1}{2} \sum_i (2 - n_i - n_i^f) \quad (9)$$

They both constitute SU(2) algebra. The main result of this letter can be states as

Theorem For bipartite lattice Λ , we have for HM, KLM. and symmetric PAM that

$$\langle \tilde{\mathbf{S}}^2 - \tilde{\mathbf{S}}_z^2 \rangle (\mu, \beta) = \langle \tilde{\mathbf{S}}_z \rangle (\mu, \beta) \text{cth} \beta \hbar \left(\frac{U}{2} - \mu \right) \quad (10)$$

where $\langle O \rangle (\mu, \beta) = \text{Tr} O \exp(-\beta K) / \text{Tr} \exp(-\beta K)$, $K = H - \mu N$, $N = \sum_{i\sigma} n_{i\sigma}$ for HM and KLM or $\sum_{i\sigma} (n_{i\sigma} + n_{i\sigma}^f)$ for PAM.

Proof. Consider the double-time Green function $\ll \tilde{\mathbf{S}}^- | \tilde{\mathbf{S}}^+ \gg_\omega$. The evolution equation of it is[14]

$$\omega \ll \tilde{\mathbf{S}}^- | \tilde{\mathbf{S}}^+ \gg_\omega = \langle [\tilde{\mathbf{S}}^-, \tilde{\mathbf{S}}^+] \rangle + \ll [\tilde{\mathbf{S}}^-, K] | \tilde{\mathbf{S}}^+ \gg_\omega \quad (11)$$

It can be calculated directly that

$$[\tilde{\mathbf{S}}^-, K] = (2\mu - U) \tilde{\mathbf{S}}^- \quad (12)$$

Accordingly, we have

$$\ll \tilde{\mathbf{S}}^- | \tilde{\mathbf{S}}^+ \gg_\omega = -\frac{2}{\omega + U - 2\mu} \langle \tilde{\mathbf{S}}^z \rangle \quad (13)$$

Therefore, the expectation value $\langle \tilde{\mathbf{S}}^+ \tilde{\mathbf{S}}^- \rangle$ can be obtained by virtue of the fluctuation-dissipation theorem

$$\langle \tilde{\mathbf{S}}^+ \tilde{\mathbf{S}}^- \rangle = \frac{i}{2\pi} \int_{-\infty}^{+\infty} \frac{\ll \tilde{\mathbf{S}}^- | \tilde{\mathbf{S}}^+ \gg_{\omega+i\eta} - \ll \tilde{\mathbf{S}}^- | \tilde{\mathbf{S}}^+ \gg_{\omega-i\eta}}{\exp \beta \hbar \omega - 1} d\omega \quad (14)$$

Using $\lim_{\eta \rightarrow 0} \frac{1}{x \pm i\eta} = \mathcal{P} \frac{1}{x} \mp i\pi \delta(x)$, we have

$$\langle \tilde{\mathbf{S}}^+ \tilde{\mathbf{S}}^- \rangle = -2 \langle \tilde{\mathbf{S}}^z \rangle \frac{1}{\exp \beta \hbar (2\mu - U) - 1} \quad (15)$$

On the other hand, we have $\tilde{\mathbf{S}}^2 - \tilde{\mathbf{S}}_z^2 = \frac{1}{2}(\tilde{\mathbf{S}}^+ \tilde{\mathbf{S}}^- + \tilde{\mathbf{S}}^- \tilde{\mathbf{S}}^+)$ and $[\tilde{\mathbf{S}}^+, \tilde{\mathbf{S}}^-] = 2\tilde{\mathbf{S}}_z$. Hence

$$\langle \tilde{\mathbf{S}}^2 - \tilde{\mathbf{S}}_z^2 \rangle = \langle \tilde{\mathbf{S}}^+ \tilde{\mathbf{S}}^- \rangle - \langle \tilde{\mathbf{S}}_z \rangle \quad (16)$$

Using eq.(9), one can readily reach the conclusion. Q.E.D.

Eq(15) can be employed to draw some conclusion on the electron desities in the three models. Since $\tilde{S}^z = \frac{1}{2}(\kappa N_\Lambda - N)$ where for HM and KLM, $\kappa = 1$ while for PAM, $\kappa = 2$, we have

$$\frac{1}{N_\Lambda} \langle \tilde{S}^+ \tilde{S}^- \rangle = (\kappa - \rho_e) \frac{1}{1 - e^{\beta \hbar (2\mu - U)}} \quad (17)$$

where $\rho_e := N/N_\Lambda$. From the finiteness of the l.h.s. of eq(17) we have the following generalization of the lemma in [22]

Corollary 1 Under the same assumptions of the theorem, for all the three models, we have: $\rho_e > \kappa$

if $2\mu > U$; $\rho_e = \kappa$ if $2\mu = U$ and $\rho_e < \kappa$ if $2\mu < U$.

For PAM, we can write $\tilde{\mathbf{S}} = \tilde{\mathbf{S}}_c + \tilde{\mathbf{S}}_f$. Since for a finite PAM system, we always have

$$\langle \tilde{\mathbf{S}}_c \cdot \tilde{\mathbf{S}}_f \rangle = \langle \tilde{S}_c^z \tilde{S}_f^z \rangle = 0 \quad (18)$$

because the bra and ket do not have equal number of creation and annihilation operators of the same kindred. So we have the following

Corolary 2 For PAM,

$$\langle \tilde{\mathbf{S}}_c^2 - \tilde{S}_c^{z2} \rangle = \langle \tilde{\mathbf{S}}_z \rangle \text{cth} \beta \hbar \left(\frac{U}{2} - \mu \right) - \langle \tilde{\mathbf{S}}_f^2 - \tilde{S}_f^{z2} \rangle \geq 0 \quad (19)$$

Since μ is the chemical potential (for PAM the conduction electrons and the localized electrons must share a common chemical potential because it is the total electron number instead each of the respect species is conserved), i.e. the fermi energy in the free fermion case, which is an intensive quantity, it must be a function of the particle density $\rho_e = \frac{N_e}{N_\Lambda}$ and the temperature β and the model parameters, $t, U, \dots, \mu = \mu(\rho_e, \beta, t, U, \dots)$ where N_e is the number of electrons accommodated in the lattice. Therefore, at any finite temperature, β , which is not a root of $\frac{U}{2} - \mu(\rho_e, \beta, t, U, \dots) = 0$ the expectation value $\langle \tilde{\mathbf{S}}^2 - \tilde{\mathbf{S}}_z^2 \rangle$ can not be of order N_Λ^2 as $N_\Lambda \rightarrow \infty$ while keeping ρ_e constant according to theorem 1. What about at the roots of $\frac{U}{2} - \mu(\rho_e, \beta, t, U, \dots) = 0$? For the HM on a bipartite lattice, using the complete particle-hole transform[23]

$$P c_{i\uparrow} P^{-1} = \epsilon(i) c_{i\uparrow}^\dagger, \quad P c_{i\downarrow} P^{-1} = \epsilon(i) c_{i\downarrow}^\dagger \quad (20)$$

For KLM, the complete particle-hole transform is defined by (19) together with

$$P S_i^{\pm loc} P^{-1} = -S_i^{\mp loc}, \quad P S_z^{loc} P^{-1} = -S_z^{loc} \quad (21)$$

i.e., the particle-hole transform effects a rotation of the spins. As to for PAM, the transform is defined by (19) together with

$$P f_{i\sigma} P^{-1} = -\epsilon(i) f_{i\sigma}^\dagger, \quad P f_{i\sigma}^\dagger P^{-1} = -\epsilon(i) f_{i\sigma}, \quad (22)$$

One has for all the three models

$$P K P^{-1} = H + \kappa(U - 2\mu)N_\Lambda + (\mu - U)N \quad (23)$$

Then since

$$\langle N \rangle_{\mu, \beta} = \frac{1}{Z} \frac{1}{\beta} \frac{\partial}{\partial \mu} \text{Tre}^{-\beta K} = \frac{1}{Z} \frac{1}{\beta} \frac{\partial}{\partial \mu} \text{Tre}^{-\beta [H + U(\kappa N_\Lambda - N) - \mu(2\kappa N_\Lambda - N)]} = 2\kappa N_\Lambda - \langle N \rangle_{-(\mu-U), \beta} \quad (24)$$

Therefore we always have $\langle N \rangle = \kappa N_\Lambda$ whenever $\mu = U/2$ no matter at what temperature. So $\mu = U/2$ can not determine the temperature. (This is why we often say the system is at half-filling when $\mu = U/2$. for HM). We have accordingly $\langle \tilde{S}_z \rangle = 0$ in this case and the *r.h.s.* of (10) is in fact 0/0, which should be determined by the limit $\lim_{\mu \rightarrow U/2}$. Since

$$\frac{1}{\beta} \frac{\partial}{\partial \mu} \langle N \rangle = \langle N^2 \rangle - \langle N \rangle^2 \quad (25)$$

we have

$$\lim_{\mu \rightarrow U/2} \langle \tilde{\mathbf{S}}^2 - \tilde{\mathbf{S}}_z^2 \rangle = \frac{1}{2} (\langle N^2 \rangle - \langle N \rangle^2) \quad (26)$$

Since for an ideal gas, the *r.h.s.* of (25), which is just the fluctuation squared of particle number, is of order $O(N)$, it is quite reasonable to assume the in the three models here, it is also of the order $O(N)$. Hence we have therefore a stronger conclusion than that in [24].

Corollary 3. *Under the same assumptions of the theorem, the l.h.s. of (10) can be at most of order $O(N_\Lambda)$ at any finite temperature for HM, KLM and PAM.*

As in ref. [25], eq(23) can be used to obtain a symmetry of the l.h.s. of eq(10). Since eq(24) states that

$$\rho_e(\mu, \beta) = 2\kappa - \rho_e(U - \mu, \beta) \quad (27)$$

we have immediately from (17) that

$$\frac{1}{N_\Lambda} \langle \tilde{S}^+ \tilde{S}^- \rangle(\mu, \beta) = \frac{1}{N_\Lambda} \langle \tilde{S}^+ \tilde{S}^- \rangle(U - \mu, \beta) \exp\{\beta \hbar(U - 2\mu)\} \quad (28)$$

There exists lot of forms of the l.h.s. of (17) satisfying this symmetry. For instance, $C(\beta, U)e^{-\beta \hbar(\mu - U/2)}$ and $C(\beta, U) \frac{1}{1 + e^{-\beta \hbar(U - 2\mu)}}$ (where $C(\beta, \mu)$ denotes some function). So the functional form can not be determined uniquely without further constraints.

By virtue of particle-hole transform (for PAM, ϵ is to be replaced by $(-1)^i$)

$$T c_{i\uparrow} T^{-1} = \epsilon(i) c_{i\uparrow}^\dagger, \quad T c_{i\downarrow} T^{-1} = c_{i\downarrow} \quad (29)$$

$$T f_{i\uparrow} T^{-1} = -\epsilon(i) f_{i\uparrow}^\dagger, \quad T f_{i\downarrow} T^{-1} = f_{i\downarrow} \quad (30)$$

under which the spin and pseudo-spin operators transform into each other [9].

$$T(S^+, S^-, S_z)T^{-1} = (\tilde{S}^+, \tilde{S}^-, \tilde{S}_z), \quad T(\tilde{S}^+, \tilde{S}^-, \tilde{S}_z)T^{-1} = (S^+, S^-, S_z) \quad (31)$$

One can obtain the knowledge of spin of the transformed model from the known knowledge of pseudo-spin of a given model [24]. From the theorem we know that at half filling, $\langle \tilde{S}_z \rangle = 0$, therefore we

always have $\langle \tilde{\mathbf{S}}^2 - \tilde{S}_z^2 \rangle = 0$ at any $\beta \neq \beta_c$, this agrees with the Corolary 2 in [5]. It was shown that[22] at half-filling for HM, no ODLRO is exhibited for on-site electron pairs in the translational invariant case for both positive and negative U . Yet, away from half-filling, it seems that theorem 1 disagrees with the theorem 1 of [9] since that theorem asserts that for negative U Hubbard model and some special ρ_e , the expectation value $\langle \tilde{\mathbf{S}}^2 - \tilde{S}_z^2 \rangle$ at ground state can be of order N_Λ^2 . But the special ρ_e was given *ad hoc* and was not determined by the grand canonical equilibrium.

As a by-product of the complete particle-hole transform, we have also the following

Corollary 4. *For the three models considered under the same assumptions as in the theorem, at half-filling, i.e. $\mu = U/2$, one has $\langle S_{x,z} \rangle = 0$*

Proof Since under the complete particle-hole transform, $PS_{x,z}P^{-1} = -S_{x,z}$, we have

$$\langle S_{x,z} \rangle = \frac{1}{Z} \text{Tr} S_{x,z} e^{-\beta K} = \frac{1}{Z} \text{Tr} (-S_{x,z}) \exp\{-\beta[H + \kappa(U - 2\mu)N_\Lambda + (\mu - U)N]\} \quad (32)$$

Therefore at $\mu = U/2$, we have

$$\langle S_{x,z} \rangle = - \langle S_{x,z} \rangle \quad (33)$$

Hence one can obtain the assertion.

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